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3D-model of epitaxy on diamond-like crystal (111) surface

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3D Monte Carlo model of epitaxy growth on {111} surfaces of diamond-cubic materials is presented. In recent papers [1, 2, 3, 4] models for diamond like crystals were suggested. Giving SOS principle up one could simulate three-dimensional surface layer. Atom diffusion could take place on the surfaces with any one orientation. Elementary events in our model are diffusion, adsorption and desorption. Temperature and growth rate are responsible for the rate of 2D nuclei creation and decreasing of intensity flux is equivalent to increasing substrate temperature. So one has every reason to introduce into the model the parameter n_{dif} equal to the number of diffusion hops between two adsorption events. Binding energies E_3 and E_2 between first and second neighbors and parameters E_{1n}, E_{2n}, E_{3n} determining atom hopping probabilities to the sites of first, second and third nearest neighbors are parameters of the model crystal.

Using the experimental STM data on flat Si(111) surface [5] we chose the value of n_{dif} to fit experimental and simulated density of island at the initial stages of growth. This density is scarcely affected by other parameters of the model. With temperature and flux intensity from [5] we estimated surface diffusion energy E_{d} on Si(111) surface as follows: the number of diffusion steps between two acts of adsorption is determined by

$$n_{\mathrm{dif}} = \nu \exp(-E_{\mathrm{d}}/kT)/V, \tag{1}$$

where E_{d} is activation energy for surface diffusion (eV), V rate of growth (bilayer per second) (defined by flux intensity), ν temperature-independent vibration frequency (s^{-1}), k Boltzmann's constant, T substrate temperature (K).

Substituting in this equation experimental temperature and rate of growth and determined by simulation n_{dif} one could obtain E_{d}.

Islands density dependence on model parameter n_{dif} is presented in Fig. 1. Experimental data dependence of island density on temperature and flux intensity [5, 6] are show as well. Both for experiment and simulation temperature ranged from 680 up to 800 K and rate of growth from 0.01 to 0.15 monolayer per minute. When the simulated curve and one of the experimental points from [5] coincided E_{d} was determined. It turns out that all experimental points agree closely with simulated curve for the same E_{d}. Our estimation gives $E_{\mathrm{d}} = (1.75 \pm 0.15)$ eV. All experimental data we used were related to temperature range corresponding to the Si (111) 7×7 surface. So surface diffusion energy estimated in this work refers to this reconstructed surface. Obtained $E_{\mathrm{d}} = (1.75 \pm 0.15)$ eV is close to $E_{\mathrm{d}} = 1.9$ eV in [1] but differ dramatically from $E_{\mathrm{d}} = 0.75$ eV determined in [5]. Such distinction is associated with procedure of data treatment. In [5] E_{d} was defined from the slope of dependence islands density on temperature and flux using Venables theory [7]. In this work we determine E_{d} from correlation of absolute values of simulated and experimental island densities.

With obtained parameters simulation gave steps moving in $[11\bar{2}]$ and $[\bar{1}\bar{1}2]$ directions close to experimental ones during growth on vicinal surfaces. Surface fragment after 0.25 bilayer (BL) deposition at the temperature $T = 690$ K is shown in Fig. 2. Islands

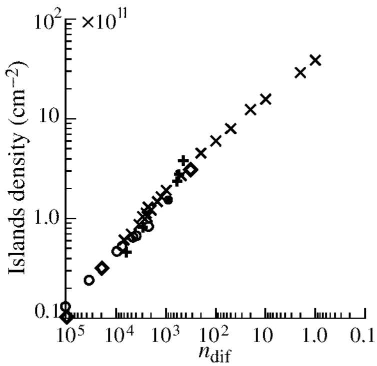

Fig. 1. Islands density dependence on model parameter $n_{\rm dif}$ ($\times\circ$) simulation results; ($\diamond$) experimental data from islands density dependence on temperature; (+) on flux intensity [ ]; ($\bullet$) experimental point from work [ ].

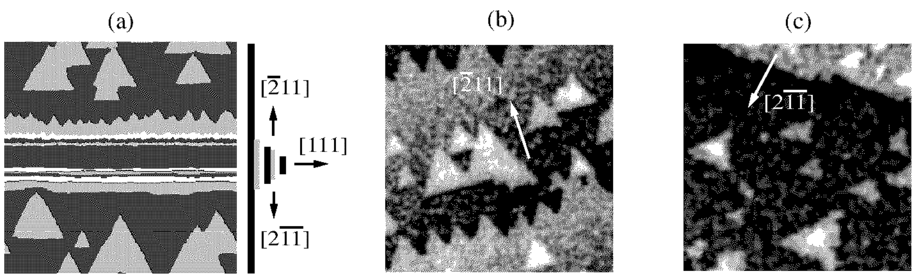

Fig. 2. Si(111) surface view at initial stage of growth. Size of the surface is 300 × 300 lattice sites, $T = 690$ K. (a) Simulated surface after 0.25 BL deposition; on the right initial profile of the echelon like surface; (b) STM view of Si(111) surface with [$\bar{2}$11] the step after 0.25 BL deposition [ ]; (c) STM view of Si(111) surface with [2$\bar{1}\bar{1}$] the step after 0.18 BL deposition [ ].

created after 0.25 BL deposition on simulated surface are similar in sizes and shape with experimental ones [ ]. Initial surface relief represented two echelons of steps of opposite direction. It is clear that steps moving in [$\bar{1}\bar{1}$2] direction are kept flat and on steps moving in opposite direction [11$\bar{2}$] one can see sawtooth shape as it was experimentally observed [ ].

We have simulated homoepitaxy process on porous Si(111). Surface fragment with one pore is shown in Fig. 3. Cross-section of the surface before and after 5 BL deposition at temperature $T = 873$ K and high rate of growth equal 60 BL/s. For these conditions it was necessary 10 BL of silicon to be the pore completely overgrown. Simulation results of epitaxy growth on porous surface with 200 × 200 atomic sites with 16 pores at temperature $T = 873$ K and rate of growth equal 1.2 BL/s are presented in Fig. 4. The sizes of each pore are 10 BL in height and 6 atomic sites in diameter. Substrate temperature and epitaxy growth rate were chosen close to experimental ones [ ]. Top view and cross-section of the surface before and after 0.5 BL deposition one can see in Fig. 4(a,b). Increasing rate of growth up to 14 BL/s at the same temperature demonstrates continuos layer creation after deposition of 4 BL. Step density oscillations calculated during 10 BL deposition at the same temperature and two different growth rates 14 BL/s (curve 1) and 1.2 BL/s (curve 2) are demonstrated in Fig. 4(c). Comparing oscillation calculated for flat and porous surfaces one could see that for high growth rate their shapes are similar (curve 1). For low growth rate (curve 2) phase delay required for porous overgrow is noticeable. Notice that porous

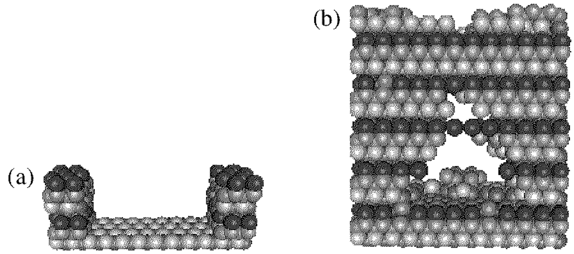

Fig. 3. Simulation of epitaxy growth on the surface with one pore; $T = 873$ K, growth rate 60 BL/s. (a) Initial surface and cross-section before deposition; (b) surface cross-section after 5 BL deposition.

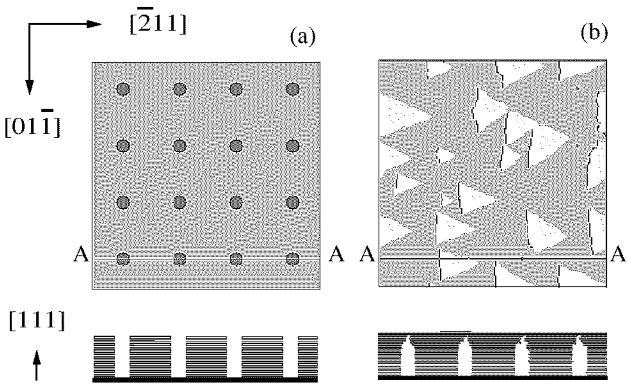

Fig. 4. Homoepitaxy simulation on porous silicon surface at $T = 873$ K. Porous diameter is 6 atomic sites, height is 10 BLs; (a) initial surface: top view and section AA; (b) surface after 0.5 BL deposition at growth rate 1.2 BL/s: top view and section AA.

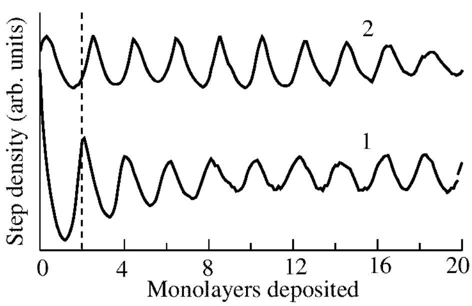

Fig. 5. Step density: curve 1—growth rate 14 BL/s, curve 2—1.2 BL/s; $T = 873$ K.

on the surface synchronize nucleation process that shows up in longer delay curve 2.

Thus the 3D-model for epitaxy on the surfaces of diamond like crystals was created. This model was successfully applied for experimental data analysis of epitaxy on (111) single crystal and porous silicon surfaces. Activation energy of diffusion hop of adatom on flat Si(111) surface was estimated from STM and simulated density of island: $E_d = (1.75 \pm 0.15)$ eV.

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